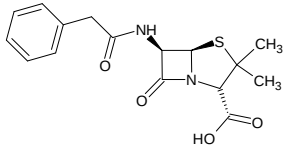
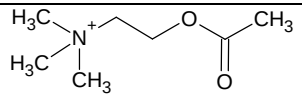
Molecules Study Guide - DRAFT

Chapter or subject	Molecule	Chemical Structure	Biochemical relevance	Physical property relevance
Alkanes	Methane	CH_4	Marsh gas, produced by methanogenic bacteria	Mp. = , Bp = , gas at STP. Because of the very low temperature on Saturn's moon Titan, methane forms clouds, rain and lakes, eroding rocks made of water ice! Also found in deep ocean deposits combined with water ice – the ice that burns!
Alkanes	Butane	$CH_3CH_2CH_2CH_3$		Liquid in lighters, gas at atm. pressure. Fits into the hydrophobic space in the helical starch structure.
Alkenes	Ethylene		Gas that causes fruit ripening and is responsible for "one bad apple spoils the bunch" and the effectiveness of fruit ripening containers. Preserve fruit in refrigerator by destroying ethylene (use $KMnO_4$)	
Alcohols, Phenols, Lipids	Capsaicin		Pain medication	Solubility, washing off tongue
Phenols, Acids & Bases	Urushiol			Washing off skin
Alkenes, lipids	Brominated vegetable oil			
Lipids	Trans fat		Implicated in heart disease	Higher melting point than cis
Lipids	Taurine		Found in bull bile. A building block of bile acids. Found in some energy	Very soluble due to zwitterion (positive and negative charge in a neutral molecule)

			drinks, but problems when mixed with alcohol. Banned in France and Japan.	
Disulfides/ proteins	Hair permanent chemicals, hair			
Thiols	Skunk thiols		Defense, oxidize with bleach or peroxide	
Lewis Structures	N_2O		anesthetic, laughing gas	Soluble in fat, so it is used as whipped cream propellant. When expelled, it creates the foam and whips the cream.
Lewis Structures	N_2O_4			Space shuttle fuel. When mixed with CH_3NHNH_2, it reacts to produce energy, no catalyst or spark required (called a hypergolic fuel.) This property is necessary for rocket engines that must operate outside the atmosphere, in the absence of oxygen.
Carbohydrates/ phenols	Propofol vs aromatic version		Drug metabolism	Acidity
Alkenes	Beta-carotene		Vision	Conjugation
Alkenes	Lycopene		Prostate health	Conjugation
Alkenes, Chirality	Menthol, carvone, other spices		Terpenes. Enantiomers of carvone have different flavors (mint vs. rye)	
Chirality	Omeprazole, S-omeprazole		Drug enantiomers often have different biological properties, “chiral switch” strategy	
Aromatics,	Benzene		Carcinogen	Aromatic stacking as a type of London force

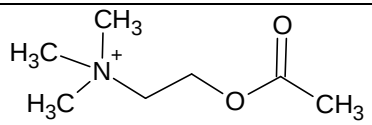
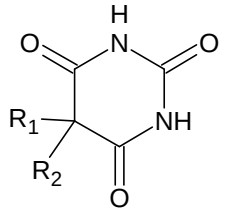
DNA				
Alcohols, enzymes	Ethanol		Alcohol dehydrogenase, some asians lack enzyme, blood alcohol test	Oxygenator in gasoline
Aromatics	Sulfa drugs		Pre-penicillin antibiotic	Water solubility
Alkenes	Bilirubin		Jaundice and its treatment	Conjugation
Alkenes	Chlorophyll, heme, vitamin B12		Grass, blood pigments	Conjugation
Ethers	MTBE			Solubility in water
Chirality	Thalidomide		Enantiomer biochemical properties	
Alcohols, Proteins	Isopropanol		Denaturation by 70% but not 90%	
Aromatics	Thyroid hormone			
Alkenes	Corn borer pheromone (connection 3B		Cis/trans isomers	
Alkenes, Aldehydes	Retinal		Cis/trans isomer conversion in vision. Retinol analog research by nakanishi. Reaction of coupling aldehyde to protein	Conjugation
Alkenes	Polymers			
Aromatics	Benzo[a]anthracene		Carcinogen	
Aromatics	Food dyes (4E)			Conjugation
Ethers	Diethyl ether (5D)		Anesthetic	Flammable
Protein,	Egg white		Anti mercury poisioning treatment	

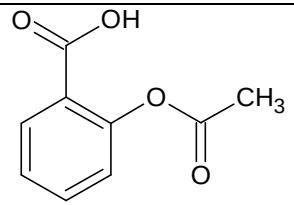
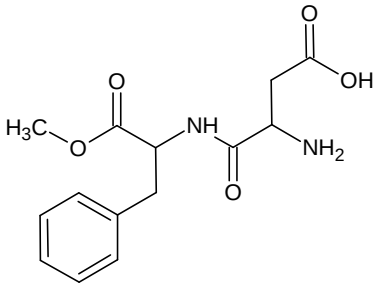
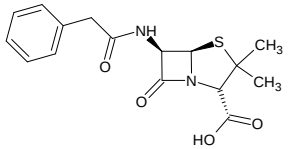
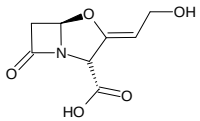
thiols				
Chirality	Ibuprofen			
	ChemConnections 9A – muscone, ionone, citronellal			
Aldehydes	Vanillin		Nice smell	Artificial vanilla vs other artificial flavors
	Soap			
Acid derivatives	Penicillin		β-Lactam antibiotic. The ring strain energy in the β-lactam ring is released when the drug reacts with an enzyme that constructs the outer membrane of the bacteria. Drug resistant strains have developed a b-lacamase enzyme.	
Carbohydrates	Xylulose			
	Hyaluronic acid			
	Heparin			
	Amylose, amylopectin, glycogen			
Carbohydrates	Corn syrup		Made by hydrolysis of sucrose followed by invertase	
Lipids	Arachidonic acid		Cyclooxygenase converts it to leukotrienes	
	Leukotrienes, prostaglandi			

	ns			
	Steroid ring parent		Hans Selye's house, stress steroid research	
Acid derivatives	Acetylcholine		Important neurotransmitter, which is hydrolyzed by the enzyme acetylcholine esterase to "turn off the message" and prepare the nerve for another signal. Inhibitors of this enzyme are important drugs and poisons.	Quaternary ammonium is always positively charged so the molecule is very soluble in water.
Acid derivatives	Barbituates			
Alkanes	Tetracycline, tricyclic antidepressants			Named after the fact that it has four or three rings
Chemical structures, Metabolism	Methyl thioacrylate		Produced in urine by catabolism of ? in asparagus, responsible for smell after digesting asparagus	
Chemical structures	Diallyl disulfide		Produced by onions and allium sp. And generates sulfuric acid in eyes? Causing lacrymation	
Proteins, DNA	SAHA		This drug inhibits the activity of lysine deacetylase., anticancer agent	
DNA, Proteins, Acid derives.	Nucleosome core particle		Lysine residues that are acetylated are no longer protonated at physiological pH, so they are neutral rather than + charged. These groups therefore have less attraction for the negatively charged phosphate groups on DNA,	

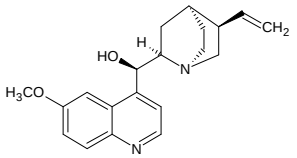
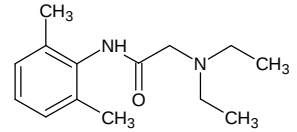
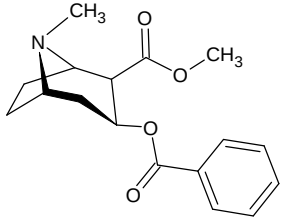
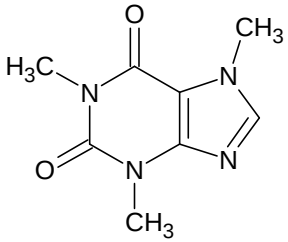
			and the DNA can unwind. Aspartic acid and Glutamic acid residues can be esterified to eliminate negative charges…	
Carbohydrates	Starch			In helical form, interior of helix is hydrophobic, allowing I2 or even butane to be absorbed by starch.
Enzymes	Carbonic anhydrase		One of the most prevalent enzymes in blood, this enzyme is responsible for catalyzing the conversion of carbonic acid to carbon dioxide, rapidly equilibrating the CO2 concentration in lungs and muscle tissues so rapid exchange of CO2 can occur.	
Drug design	Warfarin		Anticoagulant derived from coumarin, which was discovered in moldy sweet clover to cause internal hemmoraging in cattle.	
Enzymes	Furanocoumarins		In grapefruit juice, it is an inhibitor of cychrome p450(?)	
	Vanillin			
	Carvone			
	Laetrile			
	Cinnamaldehyde/Cinnamic acid			
Lipids	Solanin			
	Cholesterol			
	Digitalis			
Acids	Ammonium			

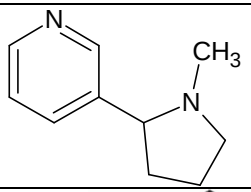
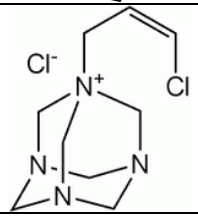
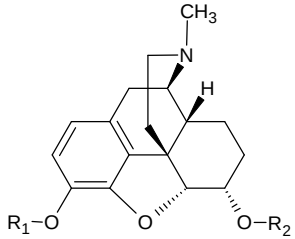
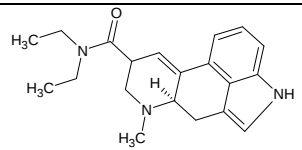
	thioglycolate			
	Palmolive detergent			
	Xylitol			
	Heparin			
	NAG-NAM			
	Lysozyme			
	Oxalic acid			

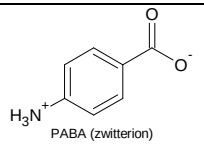
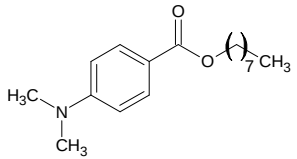
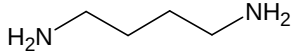
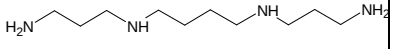
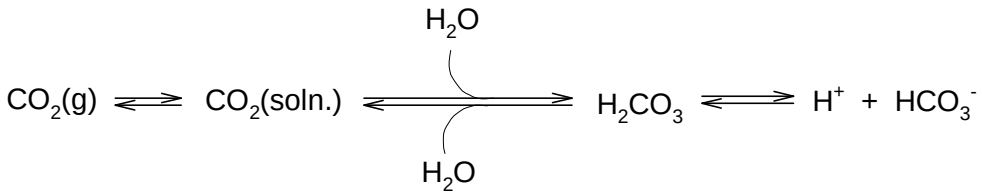
Molecule	Chemical Structure	Biochemical relevance	Physical property relevance
Acetylcholine		Acetylcholine is an important neurotransmitter. The signal is turned off when the ester bond is hydrolysed.	Quaternary ammonium ion is always + charged, which means this molecule is very soluble in water regardless of pH. A counter ion must be present as well, but is not shown in the structure at left.
Lactomer ® stitches			
Nylon		.	
Kevlar			
Protein			
Barbituates			
Acetic acid			

Acetyl salicylic acid (aspirin)			
Aspartame ®		This sugar substitute is composed of two amino acids, phenylalalanine and aspartic acid, linked by an amide bond, and a methyl ester of the phenylalanine. Hydrolysis of the ester occurs in water with heat, producing methanol. Consequently, aspartame should not be used in foods that will be heated, e.g. cake batter. Complete hydrolysis occurs in the stomach, giving methanol, phenylalanine, and aspartic acid. Children and young adults with the genetic disorder phenylketonuria (PKU) must scrupulously avoid phenylalanine in their diets, and must therefore avoid this artificial sweetener.	
Penicillin		β-Lactam antibiotic. The ring strain energy in the β-lactam ring is released when the drug reacts with an enzyme that constructs the outer membrane of the bacteria. Drug resistant strains have developed a β-lacamase enzyme.	
Clavulanic acid		This β-Lactam does not have antibiotic activity, but it is an inhibitor of the β-lactamase enzyme that gives some bacteria resistance to this class of antibiotics. The potassium salt clavulanic acid is combined with a β-lactam antibiotic to reduce the development of resistant bacteria. One example of this drug combination is Augmentin, a combination of amoxicillin and potassium clavulanate.	
Fatty acids		Fatty acids store energy and are building blocks for lipids. Enzymes create fatty acids from two-carbon building blocks, so even numbered chains are much more common in nature than odd numbered chains. Unsaturations are almost always cis, which introduces	Form micelles in water because the COOH end is soluble in water but the alkane chain is not. The Ca^{2+} and Mg^{2+} salts of fatty acids are insoluble in water and form soap scum when soap is used in hard water, which contains these ions. Cis double bonds reduce the melting point of fatty acids

		kinks into the chain.	because the kinks interrupt stacking interactions.
Acetyl-CoA			

Molecule	Chemical Structure	Biochemical relevance	Physical property relevance
Quinine		Known for over 300 years as a treatment (but not a cure) for malaria, discovery of this alkaloid from the bark of the Cinchona tree had the impact on medicine that gunpowder had on warfare. Found in non-medicinal quantities in tonic water.	Amines have a bitter taste. Amines (and alkaloids) are more soluble as the positively charged cation. Quinine is commercially available as the salt with sulfuric acid, called the sulfate. Amines also readily oxidize in air, but the protonated form is much more stable to oxidation. Tonic water fluoresces because of aromatic rings in quinine.
Lidocaine		Common local anesthetic (e.g. injection before stitches).	The HCl salt of lidocaine is more soluble in water and less susceptible to oxidation than the free amine, and this is the form used for injections.
Cocaine		Alkaloid found in coca plants. Flavoring in Coca-Cola includes extract of same plant, after cocaine has been removed. The process is carefully monitored by the FDA.	The naturally occurring protonated form is not very volatile (it has a high boiling point), making it difficult to ingest by smoking. However, the neutral amine is more volatile. "Crack" cocaine is the neutral (or "free base") form of the amine, which is more volatile and can be smoked.
Caffeine		Alkaloid found in coffee and tea.	Protonated form is more water soluble and less volatile than neutral, unprotonated form.

Nicotine		Addictive component in cigarettes, where it is normally found in the hydrochloride form.	The naturally occurring protonated form is less volatile than the neutral form. Adding ammonia (a base) to tobacco leaves releases more into the gas phase – chemical trick of cigarette manufacturers to increase the dosage of nicotine and the addictive power of a cigarette.
Quaternium-15		Preservative used in cosmetics (look for it on your shampoo bottle), it releases formaldehyde.	Example of a quaternary amine which is positively charged at any pH.
Morphine, codeine, heroin		Opium poppy contains morphine (R_1=R_2=H) and codeine (R_1=CH_3, R_2=H) , and poppy seeds contain trace amounts. Eating 2-3 poppy seed bagels can result in a positive drug test for opiates. For this reason, poppy seeds are banned in Singapore and not served on US military bases.	Heroin (R_1=R_2=$COCH_3$) is a non-naturally occurring derivative of morphine, and example of a chemical modification of a natural substance to produce a drug with different bioactivity.
Ergotamines, LSD	 LSD	Ergotamines are produced by the ergot fungus which grows on rye. These alkaloids cause ergotism, a type of poisoning. Entire towns have been poisoned when the baker's flour was contaminated. Rye must be carefully monitored to prevent formation of the ergot fungus.	A chemist created a derivative of an ergotamine, Lysergic Acid Diethylamide (LSD) which is a powerful psychotropic drug.

PABA & octyl N,N-dimethyl PABA	 PABA (zwitterion)  Octyl dimethyl PABA	Para aminobenzoic acid (PABA) or Octyl N,N-dimethyl PABA are common active ingredients in sunscreen.	The aromatic part of the molecule absorbs UV light (*due to conjugation*) and protects skin from sunburn. PABA is water soluble because it is in the zwitterions form, but octyl dimethyl PABA is much less soluble in water and therefore can be used in a sunscreen that does not wash off as easily. (A zwitterion is a neutral molecule which has a + and – charge.)
Putrescine		Responsible for the stench of dead animals, along with cadaverine and many other chemicals.	Amines can be very foul smelling compounds!
Spermine		At physiological pH, this molecule is protonated at each nitrogen, making it a polycation. This is strongly attracted to the negatively charged phosphates in DNA. Spermine is an important DNA stabilizer.	
Carbon dioxide, carbonic acid, bicarbonate, and carbonic anhydrase	 carbonic anhydrase		CO_2 equilibrium is responsible for an important pH buffer in blood. The enzyme carbonic anhydrase catalyses the equilibrium. Excess CO_2 in blood can result in excess carbonic acid and lead to low blood pH (respiratory acidosis). Hyperventilation can lower the amount of CO_2 and lower amount of carbonic acid in blood (respiratory alkalosis, “sprinters trick”) Pressure equilibrium in a soda bottle demonstrates the first reaction shown; the low pH of soda and increase in pH as CO_2 is lost demonstrates second reaction shown.
Albuterol	See Chemical Connections		